DISCOVER MORE WITH XSEDE

CHEMISTRY

Use of XSEDE Allocated Resources
Federal Fiscal Year 2019

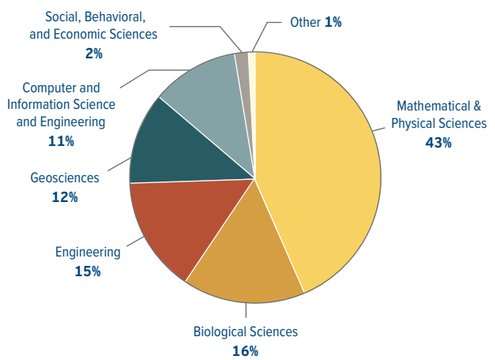
XSEDE is supported by the National Science Foundation.

The Extreme Science and Engineering Discovery Environment (XSEDE) helps the nation's most creative minds discover breakthroughs and solutions for some of the world's greatest scientific challenges. Through free, customized access to the National Science Foundation's advanced digital resources, expert consulting, training, and mentorship opportunities, XSEDE enables you to **DISCOVER MORE.**

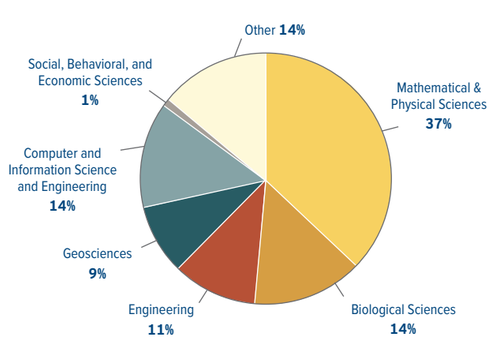
Overall Usage by NSF Directorate

NSF Directorate	Count of Projects	Count of PIs	Count of Users	Total Resource Allocation (*SUs)	Total Dollar Value	Total Resource Usage (SUs)
Mathematical & Physical Sciences	220	216	2,053	487,432,922	$7,265,582	320,769,965
Chemistry	**48**	**47**	**561**	**53,598,211**	**$859,984**	**90,698,137**
Astronomical Sciences	45	45	320	114,878,976	$1,369,856	102,796,569
Materials Research	83	81	783	170,646,656	$2,535,665	106,055
Mathematical Sciences	9	8	46	3,834,614	$79,765	3,550,365
Physics	35	35	343	144,474,465	$2,420,311	123,618,840
Biological Sciences	80	79	798	207,858,142	$3,213,225	230,788,461
Engineering	75	72	612	132,426,919	$1,790,643	121,017,568
Geosciences	59	56	494	111,562,467	$1,429,179	82,162,199
Computer and Information Science and Engineering	56	53	757	27,997,308	$478,479	21,487,867
Social, Behavioral, and Economic Sciences	10	10	57	10,878,188	$195,252	4,560,049
Other	4	4	768	681,928	$11,117	229,530,717
Total	504	490	5,539	978,837,875	$14,383,475	1,010,316,825

Number of Projects by NSF Directorate

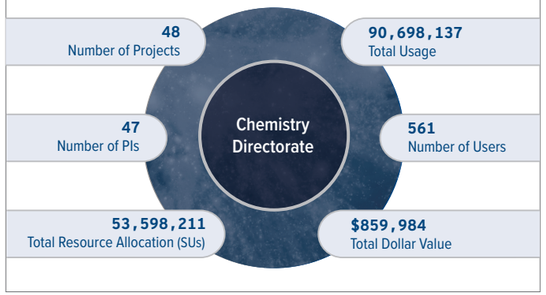


Number of Users by NSF Directorate

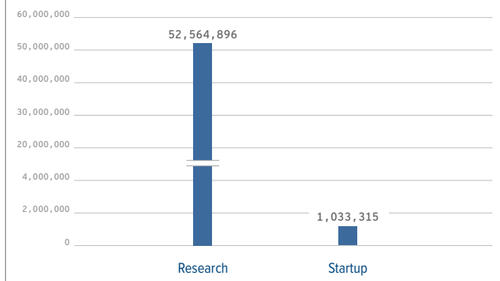


** **SU's**, or **Service Units**, are a measure of the resource allocated/used.*

XSEDE Usage for Chemistry



Chemistry User Type Breakdown



To read science successes from Chemistry, visit: *bit.ly/xsede-chemistry*

Top 10 PIs for Chemistry

PIs	Organization	Project Title	Usage (SUs)	Dollar Value
Gregory Voth	University of Chicago	Fundamental Dynamical Processes in Condensed Matter	15,432,460	$198,686
Philippe Sautet	University of California, Los Angeles	Computational Heterogeneous Catalysis	8,981,107	$191,017
Francesco Paesani	University of California, San Diego	Computational Modeling of Complex Fluids and Interfaces	7,765,822	$130,195
Sudhakar Pamidighantam	Indiana University	Science and Engineering Applications Grid (SEAGrid): A Gateway for Simulation of Molecular and Material Structures and Dynamics -Renewal	4,780,362	$93,265
Anastassia Alexandrova	University of California, Los Angeles	Dynamic Catalytic Interfaces	3,328,821	$77,062
Andreas Heyden	University of South Carolina	Multiscale Modeling of Heterogeneous Catalysts	5,367,740	$74,234
Peng Liu	University of Pittsburgh	Computational Studies of Transition Metal-Catalyzed Reactions	3,229,064	$51,879
Rigoberto Hernandez	Johns Hopkins University	Nonequilibrium Molecular Dynamics Simulations, VII	2,623,834	$50,907
Sara Mason	University of Iowa	TG-GEO160006: Density Functional Theory Calculations for Nanomaterials in Energy Applications and the Environment	2,799,194	$46,976
Dean Tantillo	University of California, Davis	Mechanisms of Bioorganic and Organometallic Crclization Reactions	2,620,376	$39,306

DISCOVER MORE
with XSEDE through:

RESOURCES
Digital services provide XSEDE users with seamless integration to NSF's high-performance computing and data resources, such as:

- High-performance computing systems
- High-throughput computing (HTC) environments
- Visualization and data analysis systems
- Large-memory systems
- Data storage
- Cloud systems
- Unique services for science gateways

SUPPORT
XSEDE's Extended Collaborative Support Services (ECSS) program offers dedicated project support for up to a year at no cost. Domain expertise is available in many areas, such as:

- Performance analysis
- Petascale optimization
- Efficient use of accelerators
- I/O optimization
- Visualization
- Science gateways
- Work and data flow systems
- Digital humanities

COMMUNITY ENGAGEMENT
XSEDE is committed to developing our workforce, fostering diversity and inclusion, and making HPC services accessible to everyone through programs such as:

- *Campus Champions*, which brings together 400+ Campus Champions at 200+ institutions to promote cyberinfrastructure in education and research
- *XSEDE EMPOWER*, an effort to expand the community by recruiting, mentoring, and enabling a diverse group of students through participating hands-on XSEDE projects
- Campus visits focused on expanding the computational science community

TRAINING
XSEDE offers a variety of training options to teach current and potential XSEDE users how to effectively utilize XSEDE services. Training classes are offered on topics such as:

- High-performance computing
- Visualization
- Data management
- Distributed and grid computing
- Science gateways

Questions? **help@xsede.org**

XSEDE is supported by the National Science Foundation.

XSEDE
Extreme Science and Engineering Discovery Environment

xsede.org

/XSEDEscience

@XSEDEscience

XSEDEscience